Methanesulfonic acid 75-75-2 | DTXSID4026422

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M. J. I	D. L.
Model	Data
110001	Bata

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 6.76 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.12e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

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Methanesulfonic acid Measured: 10.4 Predicted: 6.76

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Methylarsonic acid Measured: 1.83 Predicted: N/A

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Monosodium methanearsonate

Measured: 3.58 Predicted: N/A

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I-Taurine

Measured: 6.45e-01 Predicted: 8.59e-01

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2-Hydroxyethanesulfonic acid

Measured: 7.93 Predicted: 6.22